Mass Integration for Process Design

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November 18, 1999

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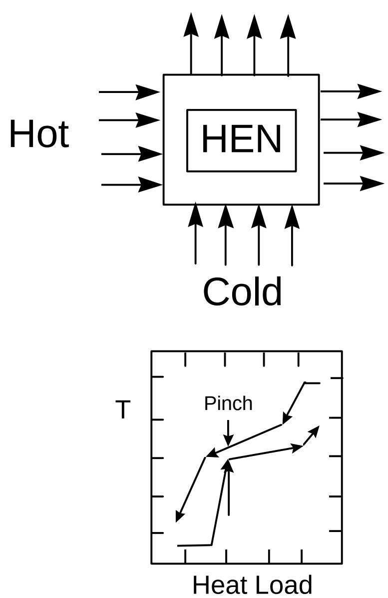
Mass Integration

- **Tool:** Minimum Mass Utility Cost for Mass Exchanger Networks with Fixed or Variable, Single Component Targets
- **Objective:** $\sum_i c_i L_i$
- **Unit Operations:** Mass Exchangers
- **Framework:** Conservation of Mass
  1st and 2nd Laws of Thermodynamics
  Mass cascades from high to low chemical potential
- **Concepts:** Mass Pinch Analysis, Composition Interval Diagrams, Mass Exchange Diagram

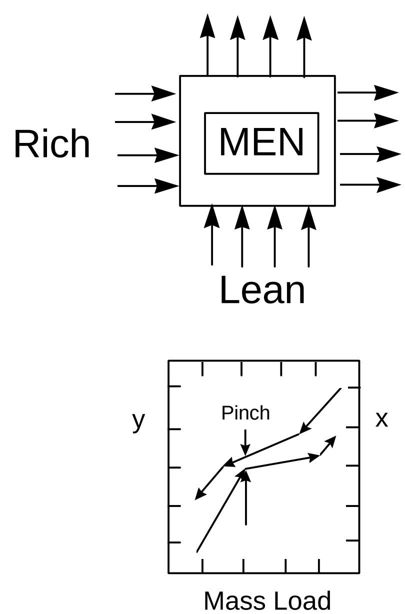
Energy Conservation

Heat Integration

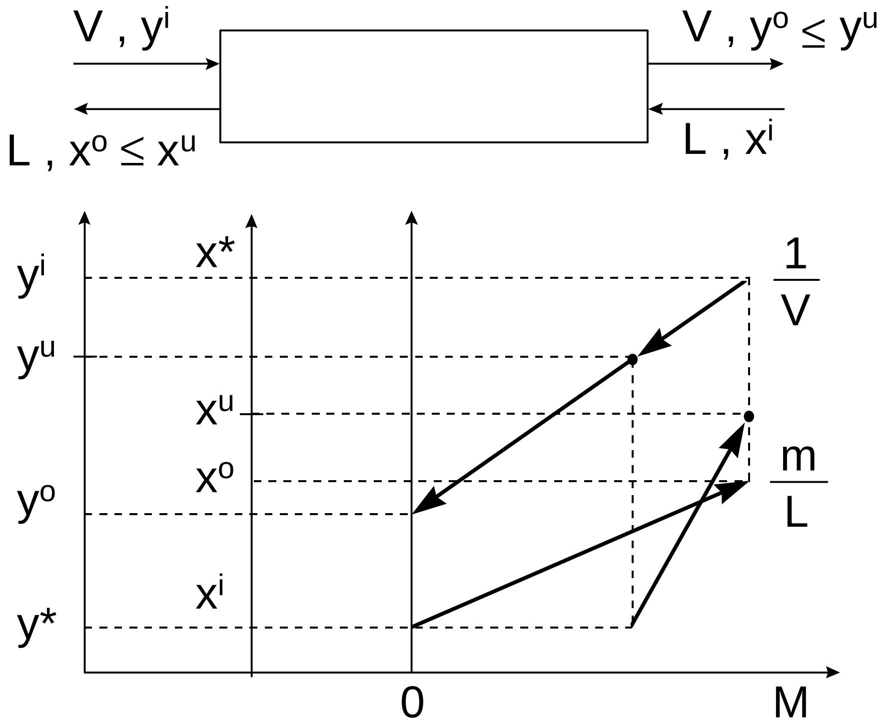


Waste Minimization

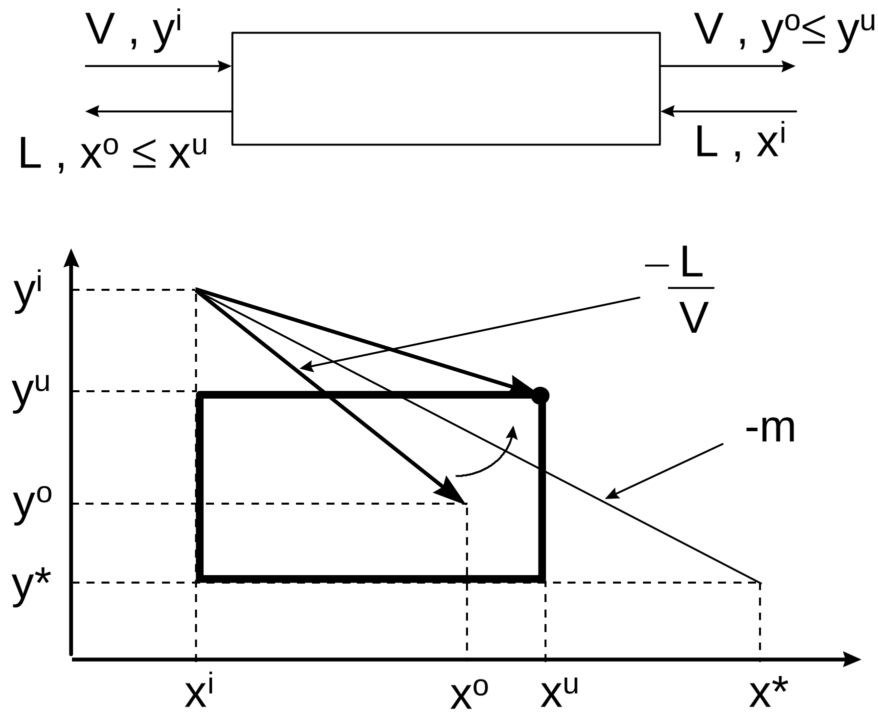
Mass Integration



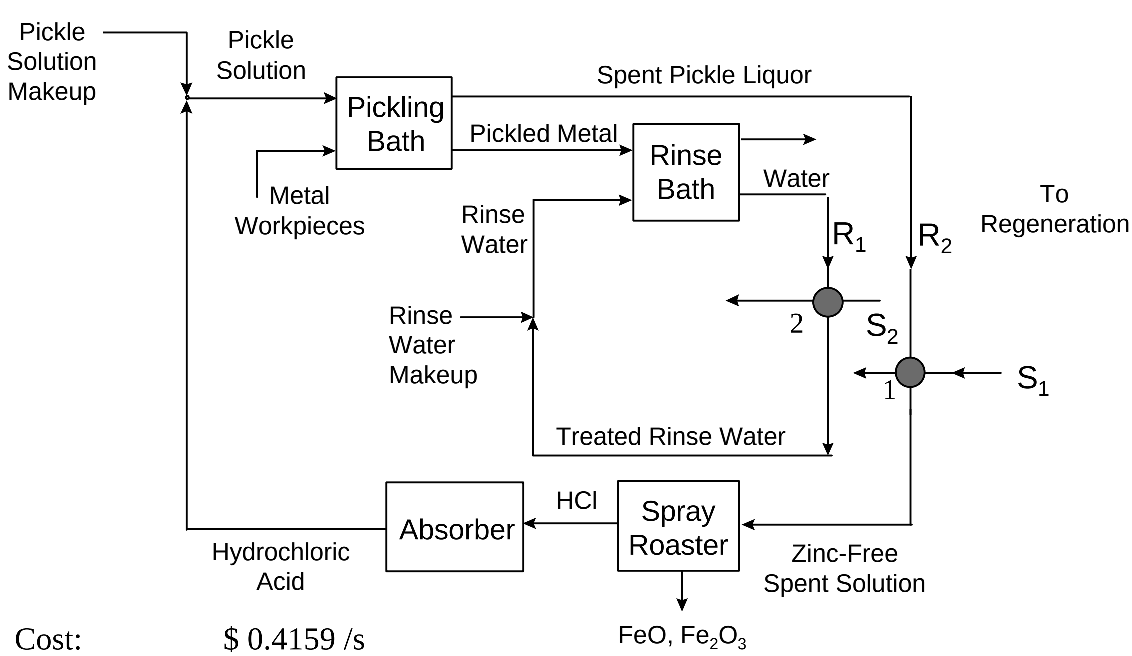
Minimum Mass Utility 1



Minimum Mass Utility 2

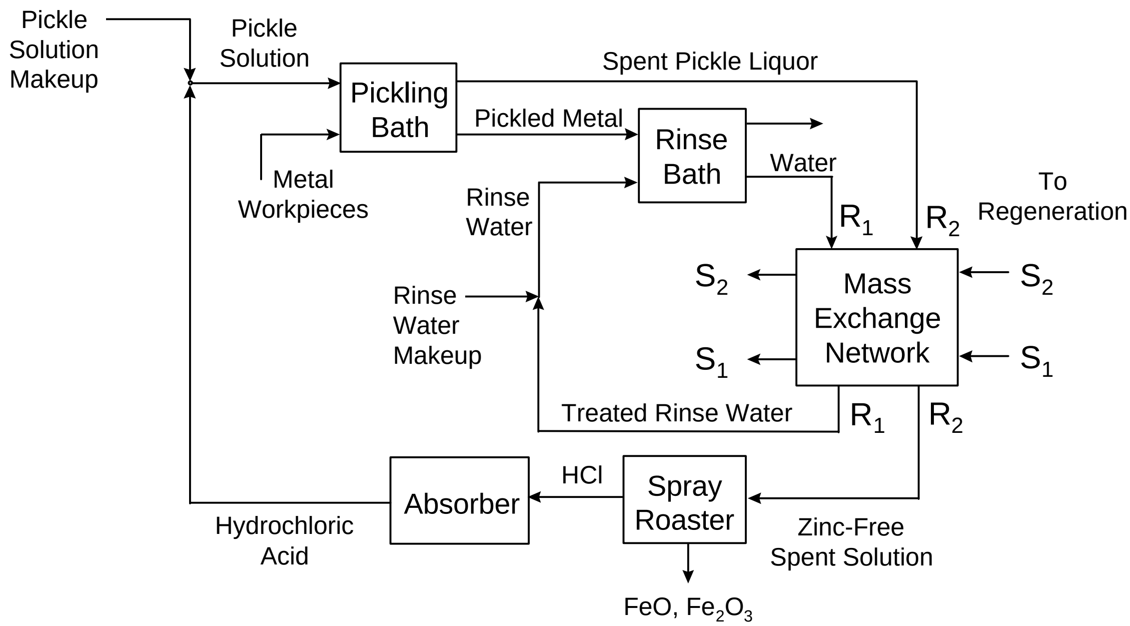


Mass Integration: Zinc Recovery - Metal Finishing Plant



Cost: $ 0.4159 /s

Mass Integration: Zinc Recovery - Metal Finishing Plant



Mass Integration: System Data

Equilibrium Data

Zinc Chloride

R (water) - S_1 (Resin) $y = 0.376\,(x+\varepsilon) + 0.0001$, $\varepsilon = 10^{-4}$

R (water) - S_2 (Phosphate) $y = 0.845\,(x+\varepsilon)$, $\varepsilon = 10^{-4}$

Input Output Data

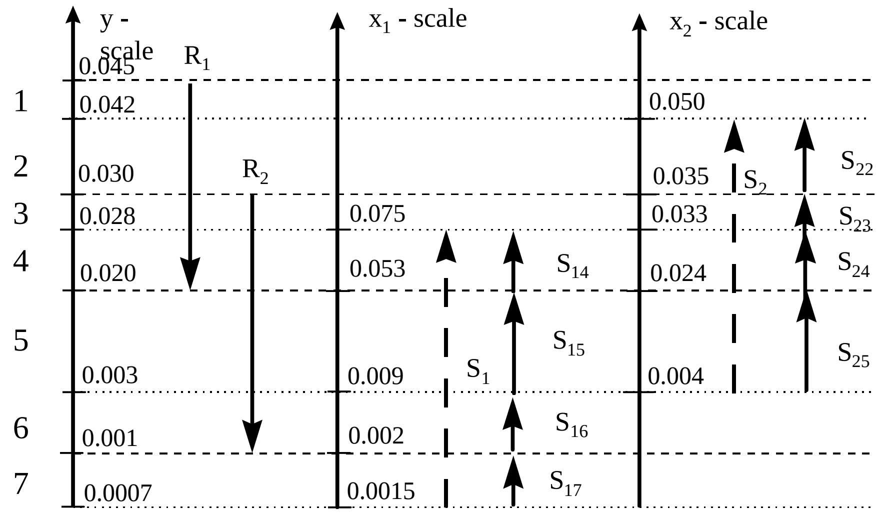
Rich Streams

	V kg/s	y^i kg/kg	y^u kg/kg
R_1	0.1	0.045	0.02
R_2	1.5	0.03	0.001

Lean Streams

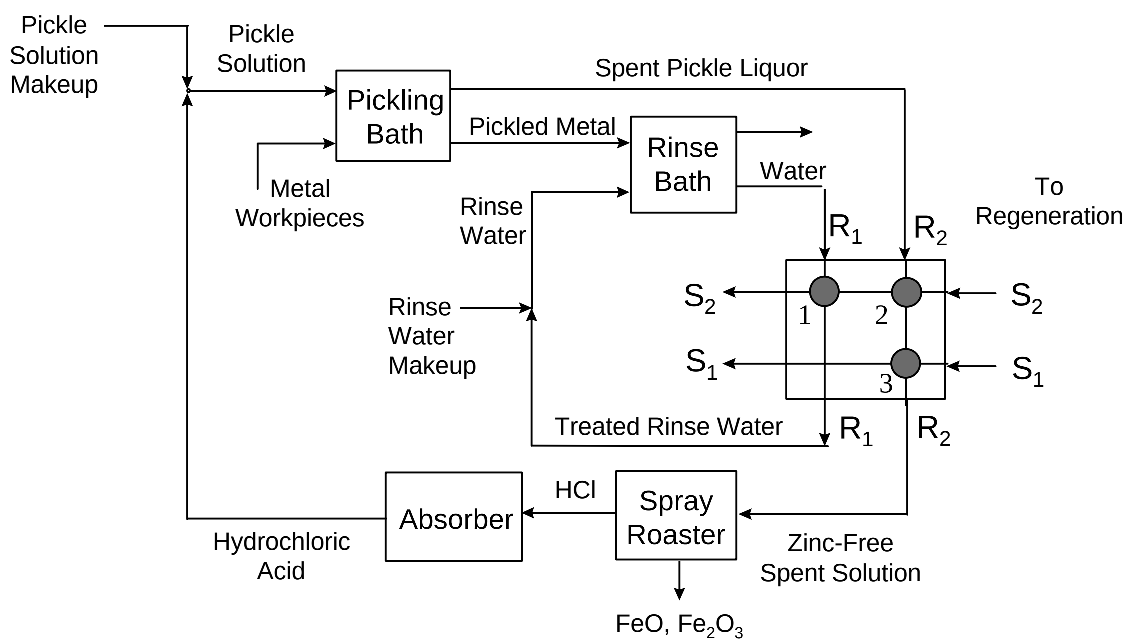
	x^i kg/kg	x^u kg/kg	c $/kg
S_1	0.0015	0.075	0.7
S_2	0.004	0.05	0.03

Mass Integration: Composition Interval Diagram



Fixed Target		Variable Target	
Cost:	\$ 0.3960 /s	Cost:	\$ 0.3594 /s
			$L_{14}=L_{15}=L_{16}=L_{17}=$ 0.5031 kg/s
Flowrates:	L_1 = 0.5615 kg/s	Flowrates:	L_{22} = 0.1028 kg/s
	L_2 = 0.1028 kg/s		$L_{23}=L_{24}=L_{25}=$ 0.2396 kg/s

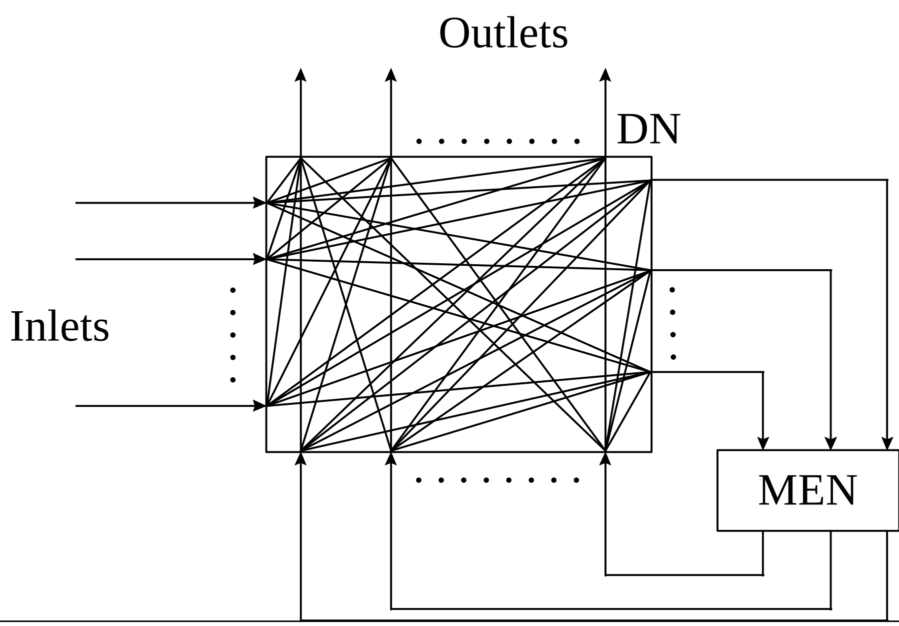
Mass Integration: Optimal Design



Multicomponent Mass Integration

- **Tool:** Minimum Mass Utility Cost for Mass Exchanger Networks with Multicomponent Targets
- **Objective:** $\sum_i c_i L_i$
- **Unit Operations:** Mass Exchangers
- **Framework:** 1st and 2nd Laws of Thermodynamics
  Infinite DimEnsional State Space (IDEAS)
  Conservation of Mass
  Mass cascades from high to low chemical potential for each component
- **Concepts:** Composition Interval Diagrams, Mass Exchange Diagrams for Each Component

Multicomponent Mass Integration: Infinite DimEnsionAl State-Space (IDEAS)



Multicomponent Mass Integration: Example

Input-Output Data

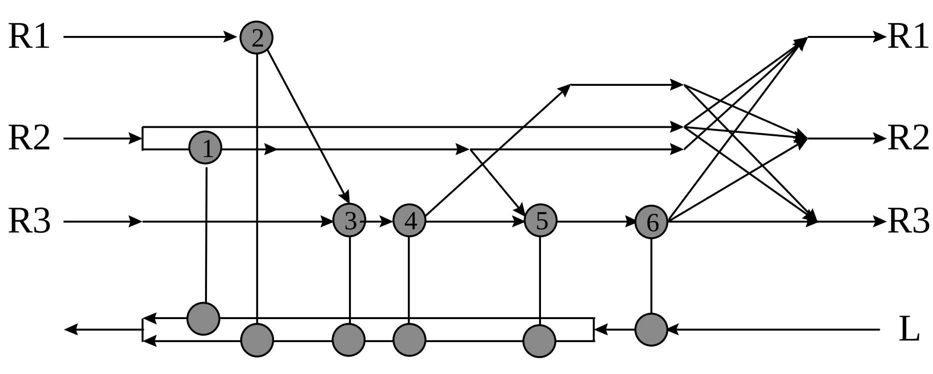
Stream	Flow	y_1^i	y_1^o	y_2^i	y_2^o
R1	0.125	0.040	0.016	0.042	0.002
R2	0.375	0.024	0.016	0.042	0.010
R3	0.125	0.024	0.016	0.074	0.010
	Cost	x_1^i	x_1^o	x_2^i	x_2^o
L	1.0	0.00	0.008	0.000	0.025

Equilibrium Data

$$y_1 = 4.0\, x_1 \quad , \quad y_2 = 2.0\, x_2$$

Multicomponent Mass Integration: Network Design

- Our recent results can identify minimum utility cost for the multicomponent MEN problem



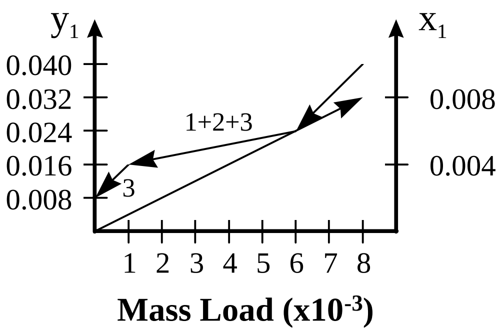
- Multicomponent Minimum Utility Cost $1.0/min

Multicomponent Mass Integration Network Data

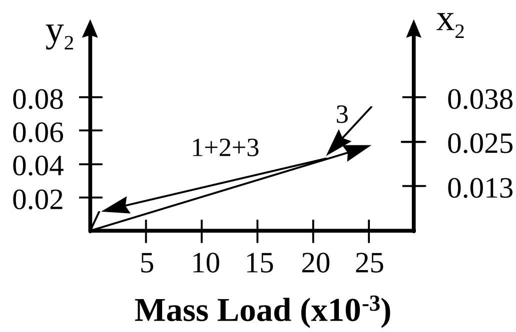
MEX	y_1^i	y_1^o	y_2^i	y_2^o	x_1^i	x_1^o	x_2^i	x_2^o	M_1	M_2
1	0.024	0.024	0.042	0.002	0.006	0.006	0.000	0.021	0.000	0.0105
2	0.040	0.024	0.042	0.074	0.006	0.010	0.037	0.029	0.002	-0.0040
3	0.024	0.024	0.074	0.010	0.006	0.006	0.005	0.037	0.000	0.0160
4	0.024	0.024	0.010	0.002	0.006	0.006	0.001	0.005	0.000	0.0020
5	0.024	0.024	0.002	0.000	0.006	0.006	0.000	0.001	0.000	0.0005
6	0.024	0.000	0.000	0.000	0.000	0.006	0.000	0.000	0.006	0.0000

Multicomponent Mass Integration: Mass Exchange Diagrams

Component 1



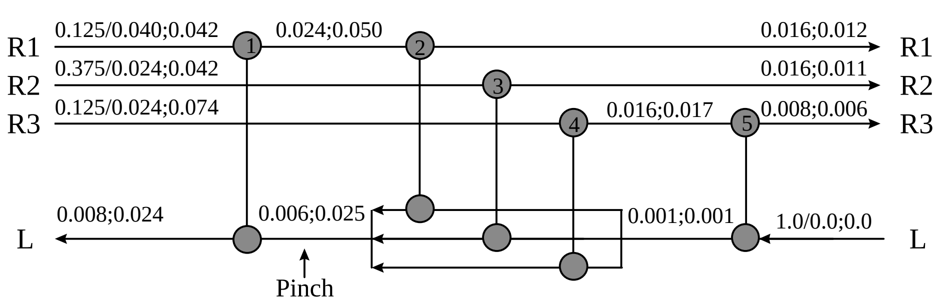
Component 2



Minimum Utility Cost
$1.0/min

Minimum Utility Cost
$1.0/min

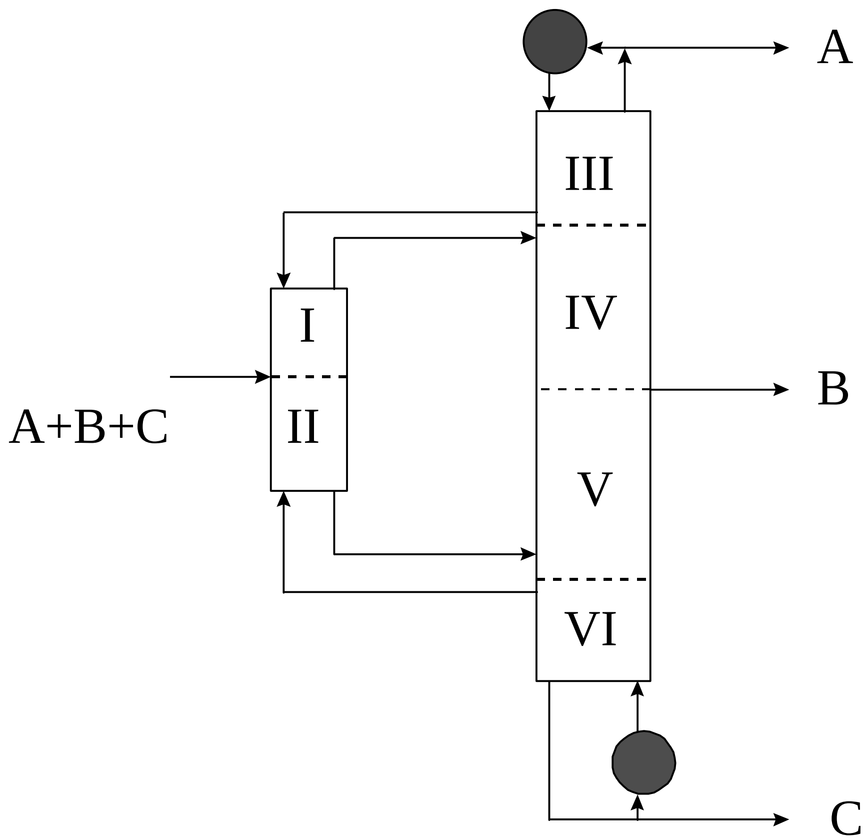
Multicomponent Mass Integration: First Component based Network Design



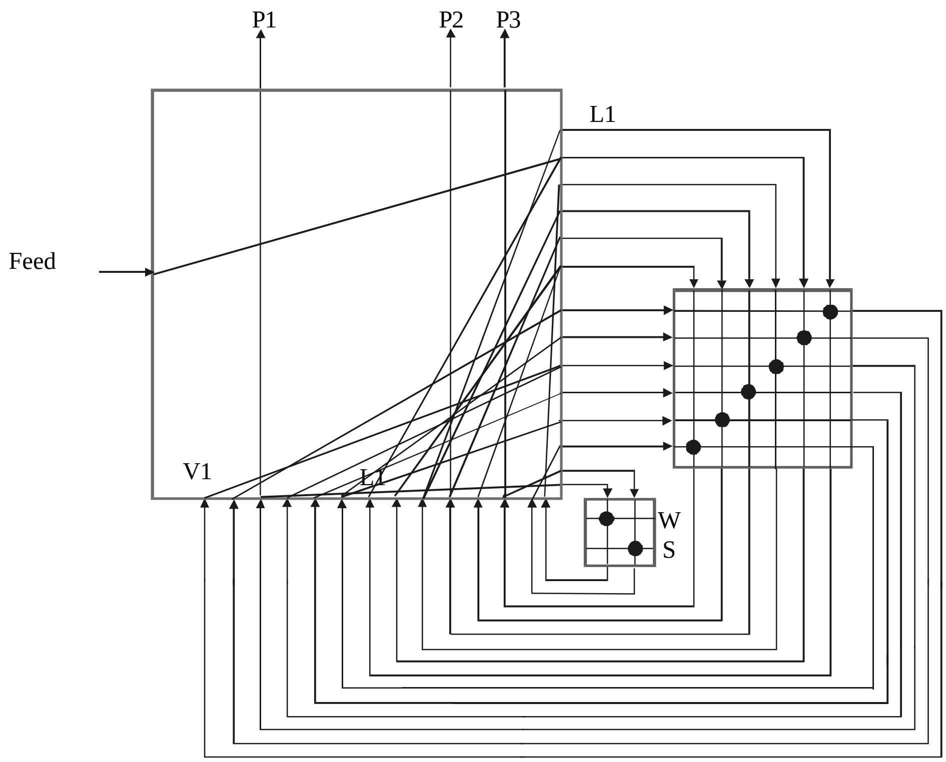
- Above network does not meet second component specifications for R1, R2
-
- Above network requires utility cost > $1.21/min to meet second component specifications

Globally Optimal Distillation Networks Minimum Utility

Petlyuk Column



IDEAS Representation of Petlyuk Column



Employed assumptions:

Process is isobaric

MEX’s incorporate equilibrium plates

HEX’s do not result in mixed phase streams

Example:

Feed: 10 kg-moles/sec: 70 mole % N_2,
30% O_2.

Distillate: 7.5 kg-moles/sec: 90% N_2

Bottoms: 2.5kg-moles/sec: 90% O_2

Constant relative Volatility: 4.173

Utility cost:

Hot utility: \$105/MJ at 92^oK

Cold utility: \$1030/MJ at 76^oK

Pressure: $1.013x10^5$ Pa

Two cases

Case 1: Feed and product streams at 78^{o}K (subcooled)

Case 2: Feed and distillate product are saturated vapor, and bottoms product is saturated liquid

Objective

Determine the *globally* minimum utility cost for a given separation using IDEAS and compare with a McCabe-Thiele design

Case 1

Distillation Efficiency, 0_d

$$0_d = \frac{|-W_{min}|}{|W_{proc}|}$$

Minimum Work of Separation, W_{min}

Difference of Gibbs Free Energy

Process work, W_{proc}

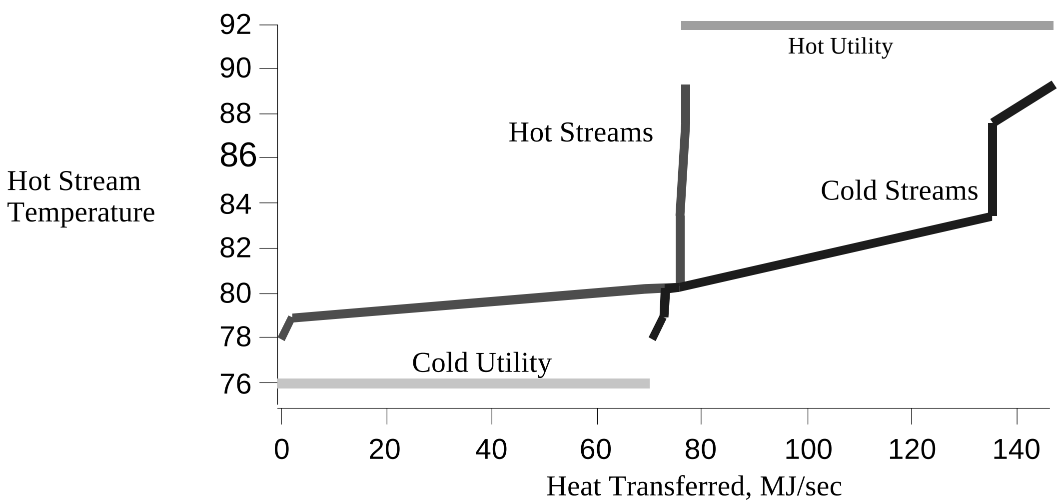
Work equavalent of heat (Carnot cycle)

$$W_{proc} = Q_{proc} \frac{(T_{proc} - T_o)}{T_o}$$

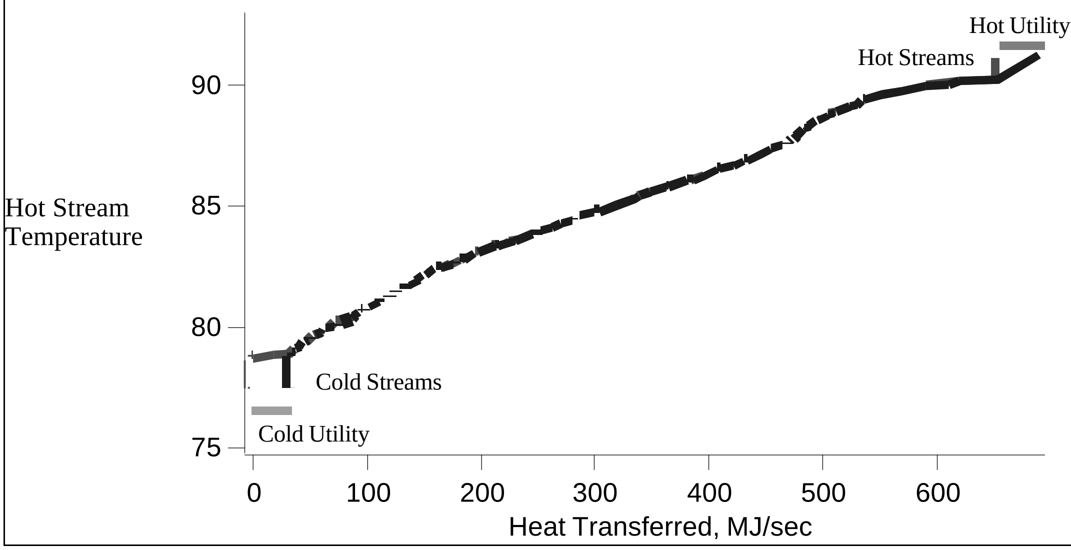
Results -- Case 1

	McCabe-Thiele	IDEAS NR	IDEAS R
Utility Use (W_{proc})	12.24	6.14	5.96
$0_d^{\ddagger}$	0.15	0.29	0.30
Cost ($/sec)	79,800	39,700	38,800

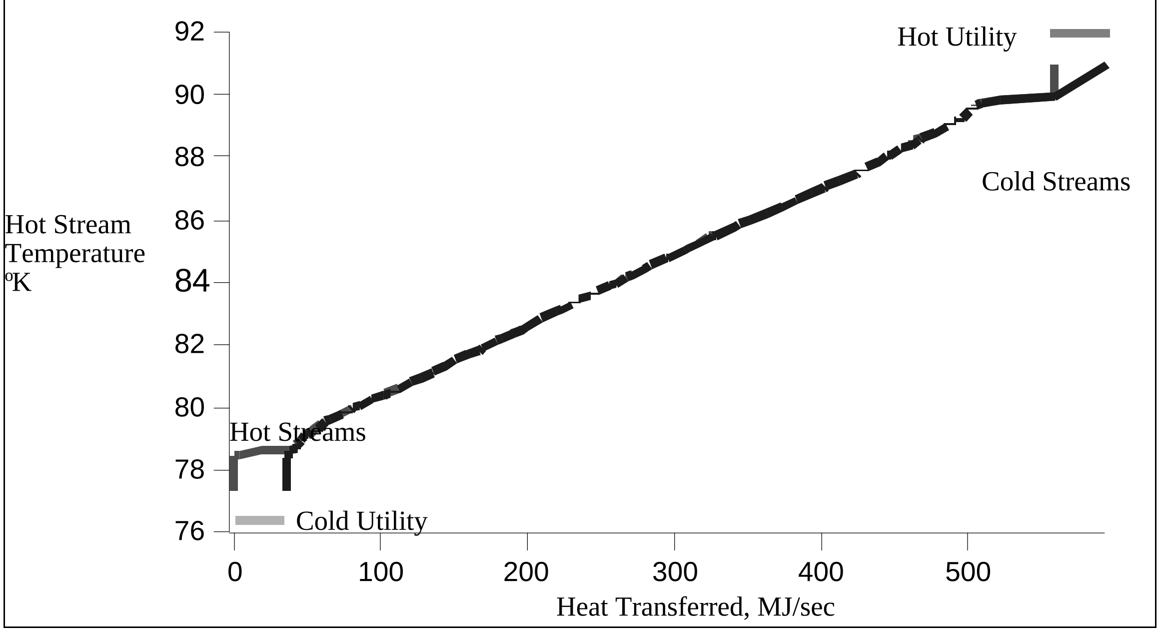
McCabe-Thiele design Temperature composite diagram



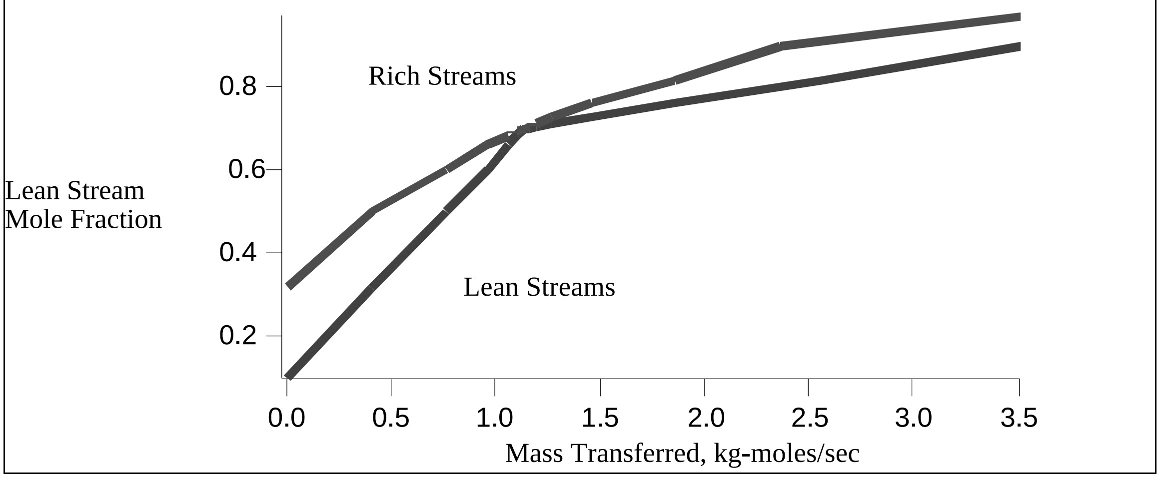
IDEAS Design
Temperature Composite Diagram Without Reverse Exchangers



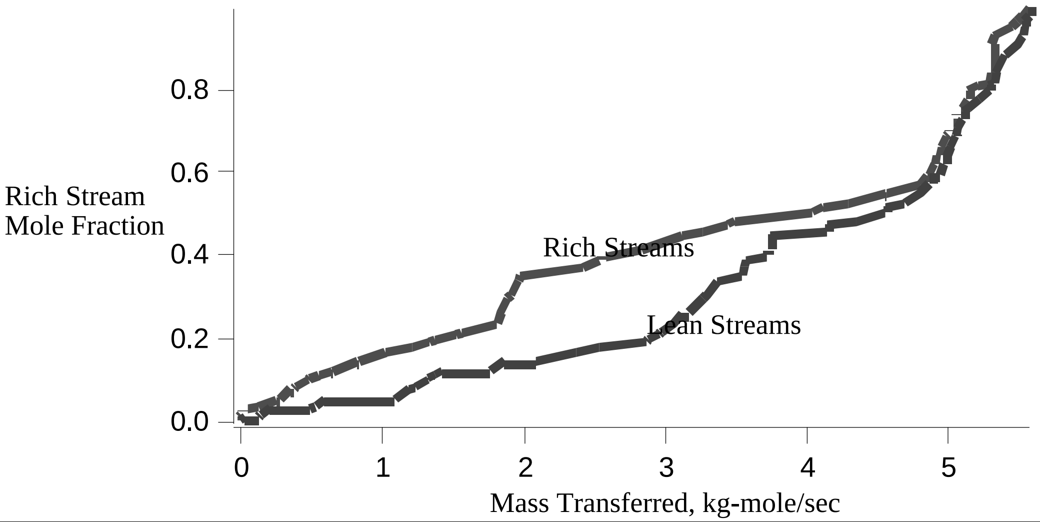
IDEAS Design Temperature Composite Diagram With Reverse Exchangers



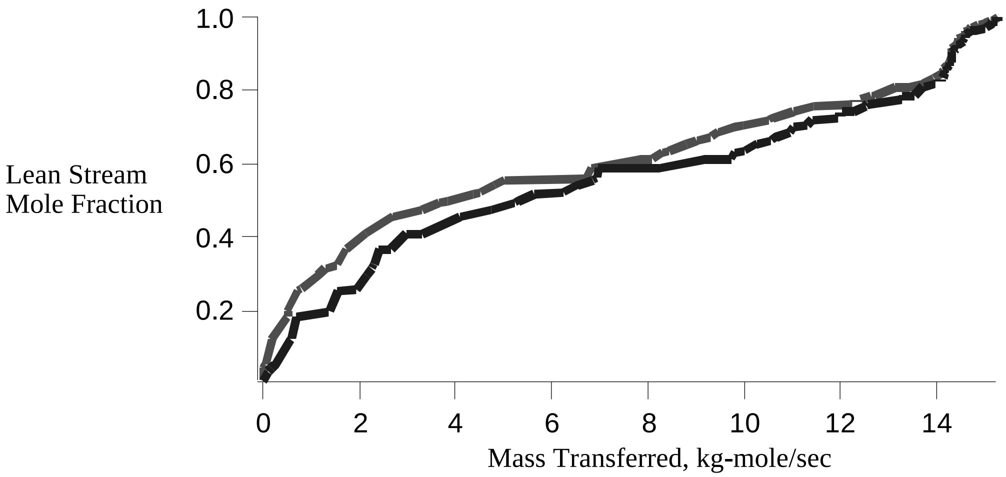
McCabe-Thiele design
Mass interval composite diagram



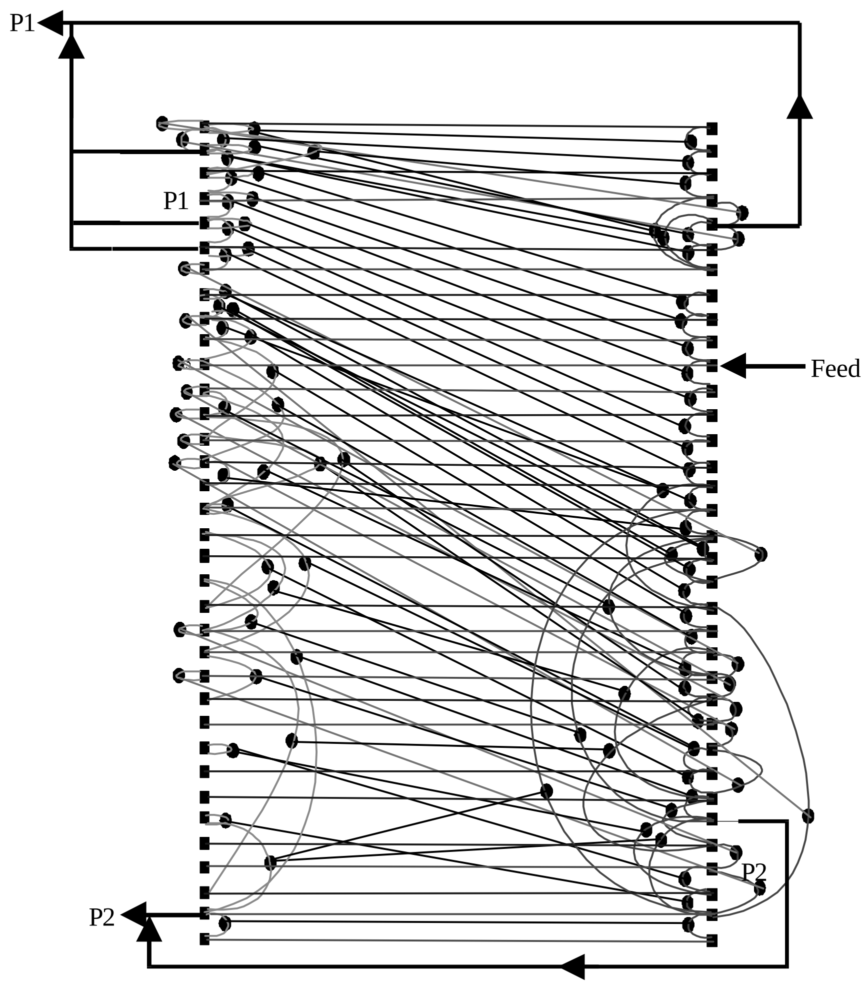
IDEAS design
mass transfer composite diagram without reverse exchangers



IDEAS design
mass transfer composite diagram
with reverse exchangers



IDEAS separation network



Case 2:

	McCabe-Thiele	IDEAS NR	IDEAS R
Hot Utility	11.74	9.11	8.76
Cold Utility	27.24	24.61	24.26
Cost ($/sec)	29,300	26,300	25,900

Globally Optimal Distillation Networks Minimum Plate Area for Fixed Utility Cost

Example:

Feed: 10 kg-moles/sec: 70 mole % N_2,
30% O_2, saturated vapor

Distillate: 7.5 kg-moles/sec: 90% N_2,
saturated vapor

Bottoms: 2.5kg-moles/sec: 90% O_2
saturated liquid

Constant relative Volatility: 4.173

Pressure: 1.013×10^5 Pa

Utility prices:

Hot utility: $105/MJ at 92°K

Cold utility: $1030/MJ at 76°K

Total utility cost: $50,000/sec

Objective

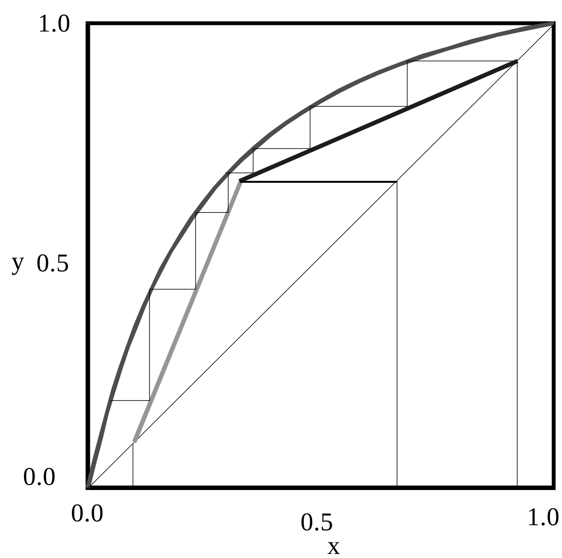
Determine the *globally* minimum plate area for a given separation and utility cost using IDEAS and compare with a McCabe-Thiele design

McCabe-Thiele design

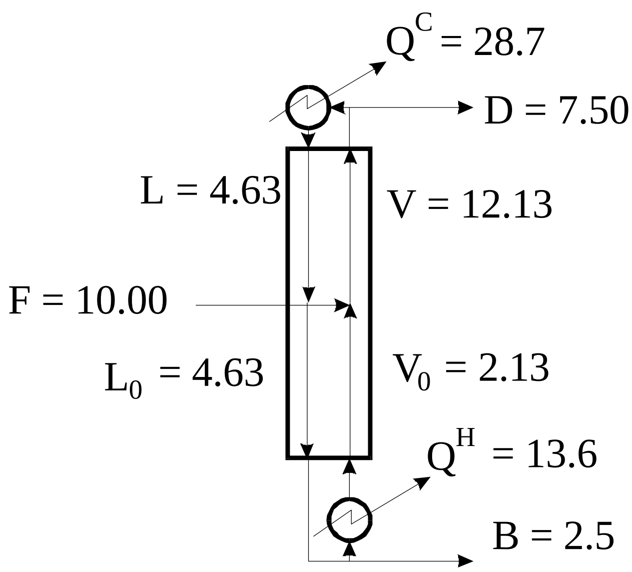
Determining heat loads

$$Fh_F + Q^H = Bh_B + Dh_D + Q^C$$

$$U = c_H Q^H + c_C Q^C$$



McCabe-Thiele design for fixed total utility cost



$$(L/V) = 1.33(L/V)_{min}$$

Results

	McCabe-Thiele	IDEAS NR	IDEAS R
Plate Area	41.1	20.3	20.3

Total Utility Cost = $50,000/sec

Globally Optimal Reaction/Distillation Networks

Motivation

- Reactor and Distillation networks impact waste generation at two levels: Processing and Recycling
- Design of such networks typically pursued through convex and/or mixed integer programs which do not guarantee global optimality.

Infinite DimEnsionAl State-space (IDEAS)

States: Composition, Enthalpy

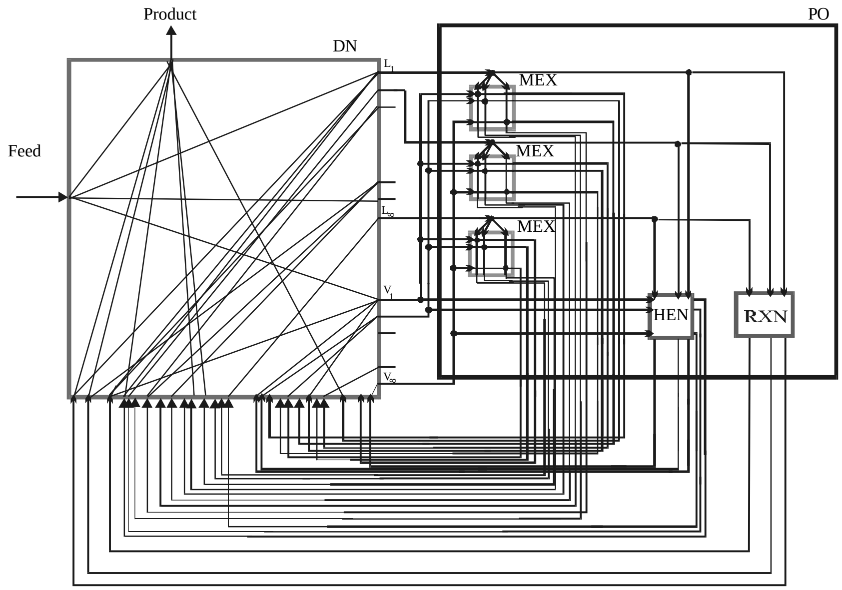
Infinite number of states

Distribution Network (DN): allows for stream mixing

Process Blocks (RXN, MEN, HEN) external to DN

Includes ALL possible designs

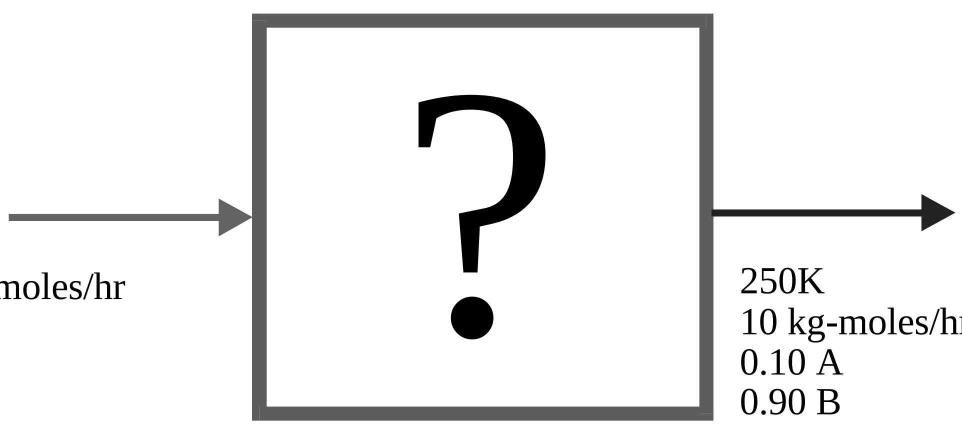
Convex Programs: Local optima are global



IDEAS Representation of a Reaction/Distillation Network

Reactor/Distillation Network Synthesis

250K
10 kg-moles/hr
0.95 A
0.05 B



250K
10 kg-moles/hr
0.10 A
0.90 B

Determine the globally minimum utility cost over any complex reactor/distillation network

Assumptions:

Process is isobaric at $5.875\text{x}10^5$ Pa

MEX’s incorporate equilibrium plates

HEX’s do not result in mixed phase streams

States are feeds, products, saturated liquids/vapors

Local mixing

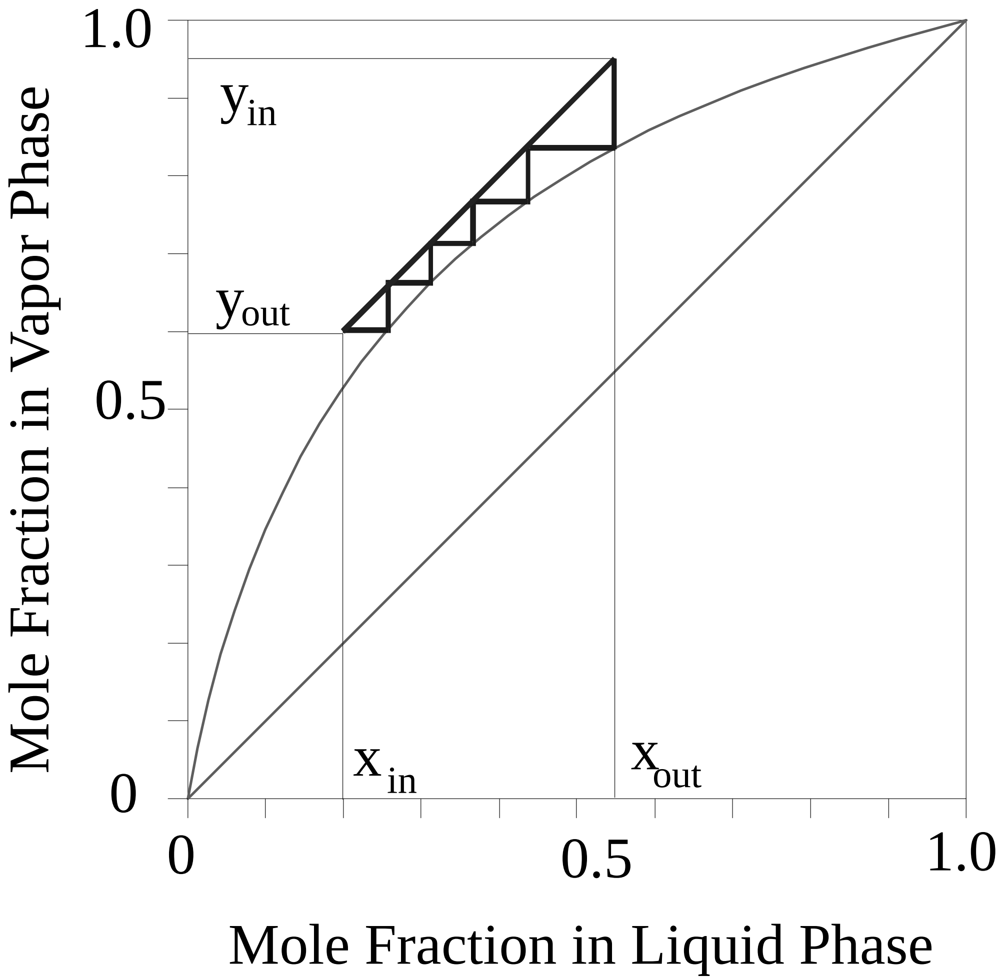
Reverse exchangers allowed

Constant relative volatility: 4.422; Chemical equilibrium constant: 1.7

Hot utility available at 92K for $105/MJ, cold utility at 76K for $1030/MJ

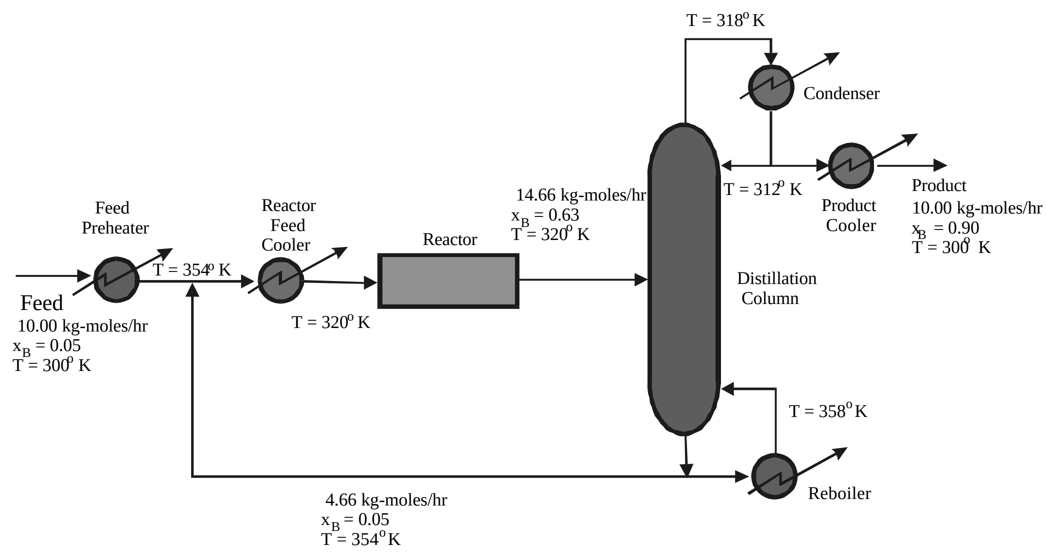
Reactors operate isothermally

Forward reaction is exothermal:) H_r = -1.62-0.0027(T-298) MJ/kg-mole



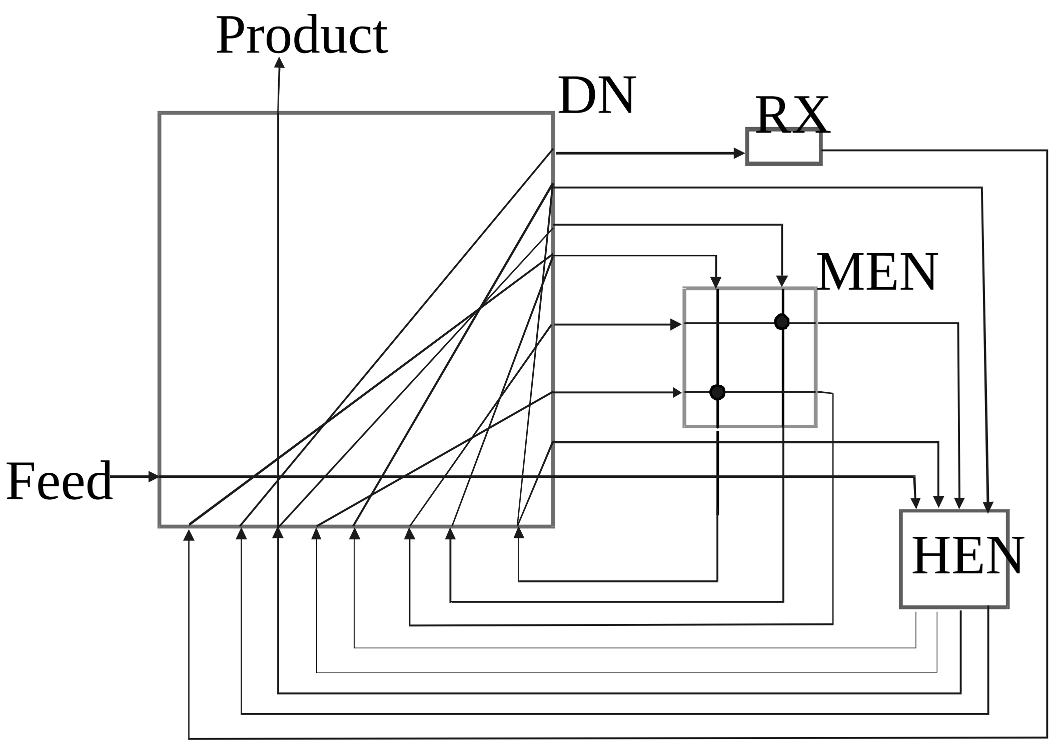
Reverse Exchangers

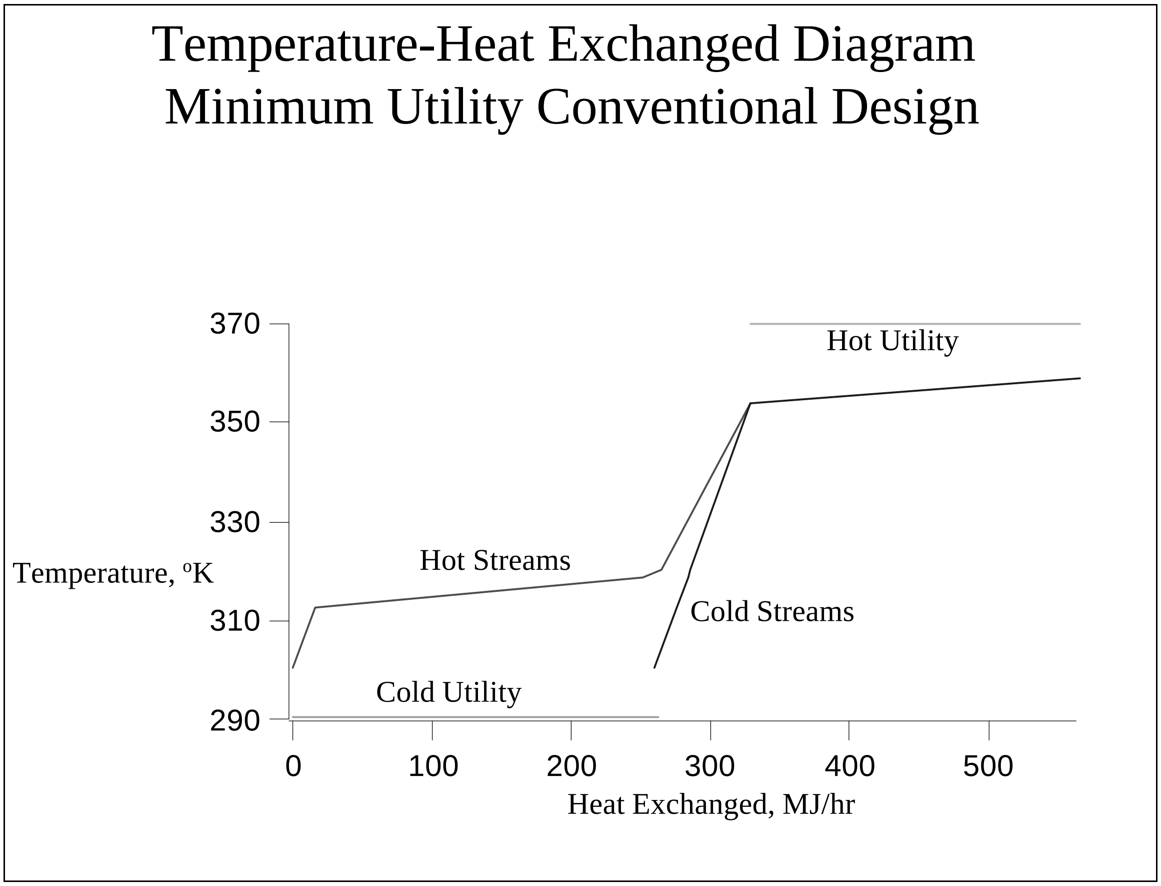
Reactor/Distillation Conventional Design Minimum Utility Design



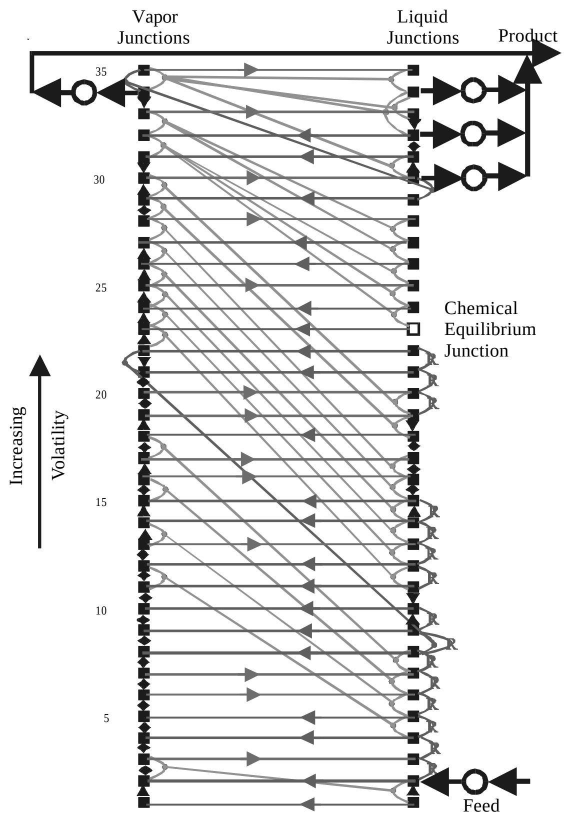
Utility Cost:
$0.773/hr

State-space representation of conventional optimal design



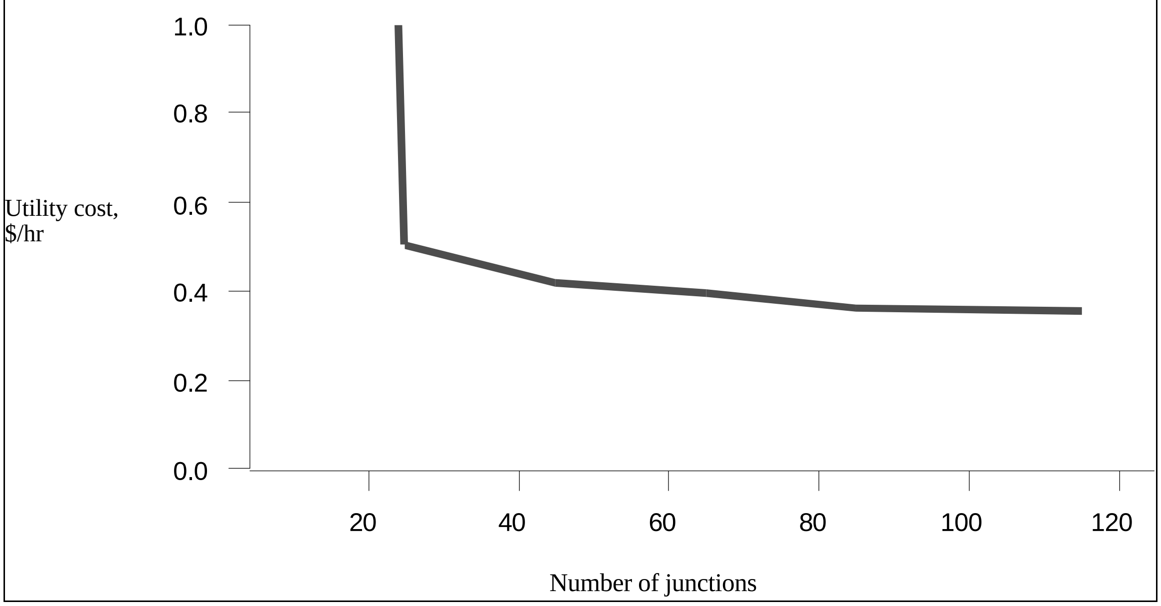

Temperature-Heat Exchanged Diagram
Minimum Utility Conventional Design
370
350
330
310
290
Temperature, °K
Hot Utility
Hot Streams
Cold Streams
Cold Utility
0
100
200
300
400
500
Heat Exchanged, MJ/hr

IDEAS Optimal Design Minimum Utility

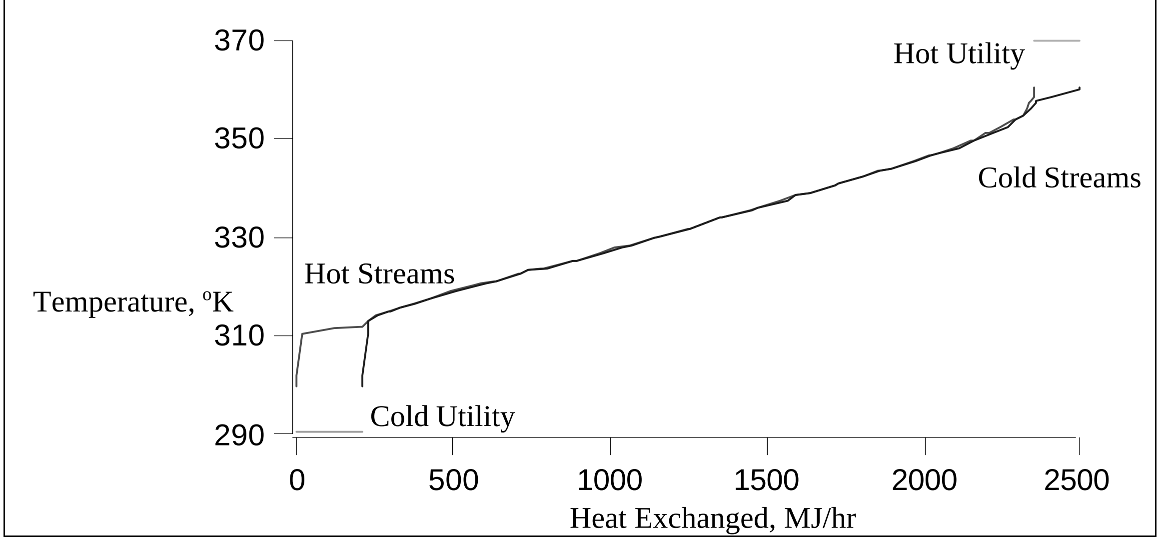


Utility Cost: $0.365/hr

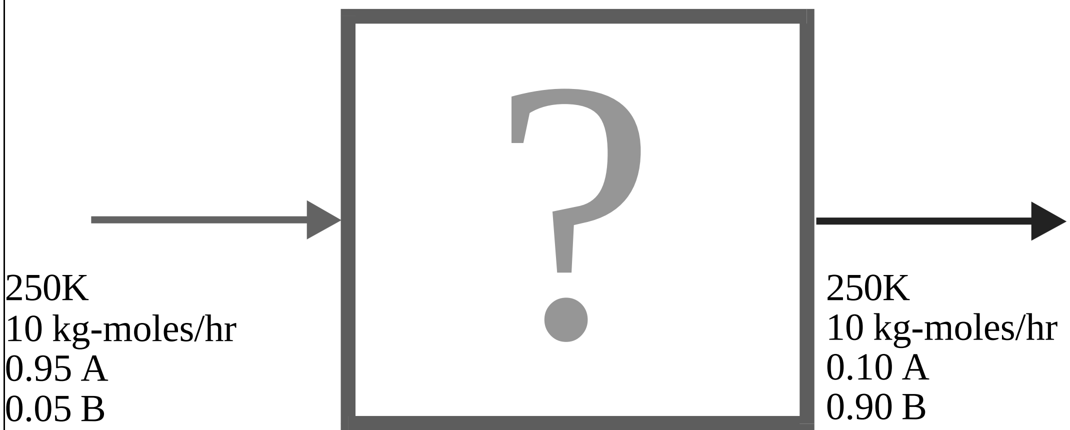
IDEAS Convergence Characteristics



Temperature-Heat Exchanged Diagram
Minimum Utility IDEAS Design



Reactor/Distillation Network Synthesis



Determine the globally minimum linear total annualized cost (TAC) over any complex reactor/distillation network

Additional Assumptions:

Capital cost of plates linearly proportional to plate area = $50/m^2

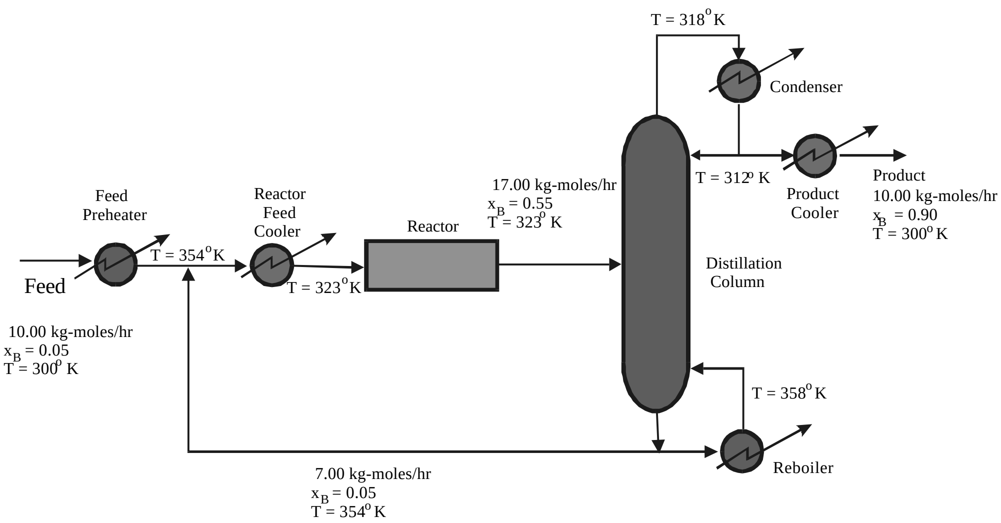
Capital cost of reactors linearly proportional to reactor volume = $100/m^3

TAC is given by

TAC = Annual utility cost + (Total capital cost)/ (Project life)

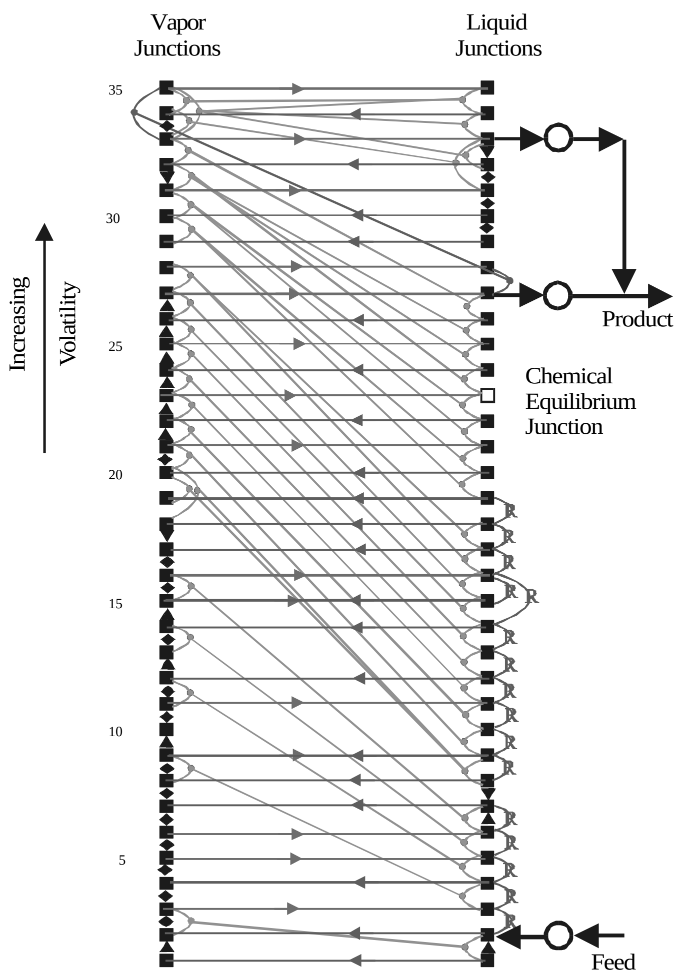
Project life = 7 years

Reactor/Distillation Conventional Design Minimum TAC Solution



LTAC: $10,358

IDEAS Optimal Design LTAC



LTAC: $6,487/yr

Conclusions

Infinite DimEnsionAl State-space (IDEAS) process representation includes all possible processes

Resulting problem formulations are convex

IDEAS designs are flexible and may be used to represent a wide variety of processes

For reaction/distillation networks, IDEAS designs have lower utility cost and TAC than conventional designs

ACKNOWLEDGEMENTS

Mahmoud El-Halwagi
Ashish Gupta
Stevan Wilson
James Drake